TITLE: Residual Scale Dependence and PDE Filters

RESIDUAL SCALE DEPENDENCE AND PDE FILTERS

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1. Introduction

In [1] and [2] the filter operation acting upon nonlinear partial differential equations (PDE) is examined by way of a PDE filter on a domain involving space/time and an additional dimension associated with a space scale parameter. Under this approach it is possible to obtain an estimate for the error associated with the equations satisfied by the filtered solutions of the microscopic scale PDE given any approximation of the residuals. This provides a condition of consistency. The PDE filter approach suggests approximations for the residuals that are independent of empirical, or arbitrary, parameters.

Here the main points of [1] and [2] are presented with some additional issues addressed. An attempt is made to remain within a setting of general nonlinear PDE systems. The filtered equations of reactive turbulent flows are presented as an example.

2. Macroscopic Equations

Let $\Omega \subseteq \mathbf{R^3}$, $T = (0, t_0)$ and $\eta \in I = (0, \eta_0)$, where $t_0 > 0$ and $0 < \eta_0 << 1$. Define $M \subset \mathbf{R^n}$ such that $M = \Omega \times T \times I$. If $\Omega \subset \mathbf{R^3}$ is bounded we denote the boundary of Ω by $\partial\Omega$. The summation convention of repeated upper and lower indices is adopted and for convenience the following ranges for the indicated indices should be assumed throughout: $a, b, c, d \in \{1, ..., n-2\}$; $i, j, k, l \in \{1, ..., n-1\}$; $p, q, r, s \in \{1, ..., n\}$. Here n $(= 5)$ is the dimension of M and under this convention $(x^a) = (x^a)_{1 \leq a \leq 3} = (x, y, z)$, $x^{n-1} = t$, $x^n = \eta$. Hence we write, Ω has a coordinate system (x^a), $\Omega \times T$ has a coordinate system $(x^i) = (x^a, t)$ and M has a coordinate system $(x^p) = (x^i, \eta)$. The Greek indices are within the range: $\alpha, \beta, \gamma, \delta \in \{1, ..., N\}$, and are associated with the dependent variables, u^α, where N denotes the number of dependent variables. Throughout we shall work with nondimensional variables.

The scale parameter η is defined by

$$\eta = \beta\epsilon^2/2 \tag{1}$$

where $\epsilon = l/L$ represents the ratio of the microscopic length scale l (smallest resolvable characteristic length scale) and the macroscopic length scale of the domain L. The parameter β (> 0) is chosen to control the rate of damping of fluctuations in the dependent variables. In most practical applications, ϵ represents a characteristic grid size for a (nondimensional) spatial discretization.

The set of smooth functions on M will be denoted by $F(M)$. For any $f \in F(M)$ the comma followed by a subscript $f_{,p}$ will indicate the partial derivative of f with respect to the coordinate x^p. It should be noted that much of the work that follows could be relaxed by replacing the smoothness condition to one of differentiability of some finite order. It will be useful to introduce a subset $\widehat{F}(M) \subset F(M)$ which is defined as follows:

Definition 1. Any $f \in \widehat{F}(M)$ has the following properties:
(i) $f \in F(M)$
(ii) For any $u^\alpha \in F(M)$, $f = \mathrm{fn}(u^\alpha, u^\alpha_{,i}, u^\alpha_{,ij})$.

Property (ii) of the definition states that any member of $\widehat{F}(M)$ can be expressed in a functional form explicitely independent of x^p, $u^\alpha_{,n}$ and $u^\alpha_{,np}$. It should be pointed out that $\widehat{F}(M)$ is introduced here only to avoid some notational difficulties. In [2] the ideas that follow are more conveniently developed in the setting of contact manifolds where some of the restrictions introduced here can be avoided.

For any $u^\alpha \in F(M)$ let $\varphi^\alpha \in F(M)$ be defined by

$$\varphi^\alpha = (\frac{\partial}{\partial\eta} - L)u^\alpha \tag{2}$$

where L is an elliptic differential operator on Ω.

Define the vector field operator

$$U = L(u^\beta)\partial_\beta + (L(u^\beta))_{,i}\partial^i_\beta + (L(u^\beta))_{,ij}\partial^{ij}_\beta \tag{3}$$

with the notation

$$\partial_\beta = \frac{\partial}{\partial u^\beta}, \quad \partial^i_\beta = \frac{\partial}{\partial u^\beta_{,i}}, \quad \partial^{ij}_\beta = \frac{\partial}{\partial u^\beta_{,ij}} \tag{4}$$

A calculation shows that

$$(\frac{\partial}{\partial\eta} - U)f = Wf, \qquad f \in \widehat{F}(M) \tag{5}$$

where

$$W = \varphi^{\alpha}\partial_{\alpha} + \varphi^{\alpha}_{,i}\partial^{i}_{\alpha} + \varphi^{\alpha}_{,ij}\partial^{ij}_{\alpha} \tag{6}$$

The PDE filter is defined as follows:

Definition 2. Any $u^{\alpha} \in PDEF\{L, \tilde{f}^{\alpha}, \tilde{u}^{\alpha}\}$ has the following properties:

(i) $u^{\alpha} \in F(M)$, $\tilde{u}^{\alpha} \in F(\Omega \times T)$ and

$$u^{\alpha}|_{\eta=0} = \tilde{u}^{\alpha} \tag{7}$$

(ii) $L : F(M) \to F(M)$ is an elliptic operator on Ω and

$$(\frac{\partial}{\partial \eta} - L)u^{\alpha} = 0, \qquad (x^{p}) \in M \tag{8}$$

(iii) $\tilde{f}^{\alpha} \in \widehat{F}(M)$ vanishes at $\eta = 0$, i.e.

$$\tilde{f}^{\alpha}|_{\eta=0} = \tilde{f}^{\alpha}(\tilde{u}^{\beta}, \tilde{u}^{\beta}_{,i}, \tilde{u}^{\beta}_{,ij}) = 0 \tag{9}$$

In Definition 2 the $\tilde{u}^{\alpha}(x^{a}, t)$ are exact solutions of the equations that describe the system at the microscopic scale. These are expressed in the form of the PDE system (9) defined on $\Omega \times T$. ¿From the prescribed data $u^{\alpha}|_{\eta=0} = \tilde{u}^{\alpha}(x^{a}, t)$ we can generate a one parameter family of fields $u^{\alpha}(x^{a}, t, \eta)$ on M by integrating (8) with respect to the scale parameter η. The operator L must be chosen such that the integration of (8), with respect to η, will damp out fluctuations in each $\tilde{u}^{\alpha}$ that cannot be resolved on each scale associated with the parameter η. We will refer to $u^{\alpha}(x^{a}, t, \eta)$ for $\eta > 0$ generated by (8) as the filtered fields associated with solutions of the system of PDE (9). The existence of each $\tilde{u}^{\alpha} \in F(\Omega \times T)$ (coupled with suitable boundary conditions for the filtered fields on $\partial\Omega$ if Ω is bounded) is sufficient to guarantee the existence of the filtered fields $u^{\alpha} \in PDEF\{L, \tilde{f}^{\alpha}, \tilde{u}^{\alpha}\}$.

An effective filter in its simplest form can be obtained using the space Laplace operator

$$L = \delta^{cd} \frac{\partial^{2}}{\partial x^{c} \partial x^{d}} \tag{10}$$

where $\delta^{cd} = 1$ if $c = d$ and $\delta^{cd} = 0$ if $c \neq d$. For demonstration purposes we assume (10) throughout. It should be noted that here we are employing space filters. Definition 2 could be easily modified to include space and/or time filters. The simplest time only filter can be obtained by setting $L = \partial^{2}/\partial t^{2}$.

If $\Omega = \mathbf{R^{3}}$ and each $\tilde{u}^{\alpha} \in F(\Omega \times T)$ is bounded on $\Omega \times T$ then the filtered fields obtained from the integration of (8) with respect to η subject to the initial data (7) yields the Gaussian filter

$$u^\alpha(x^a,t,\eta) = \int_\Omega G(x^a - z^a,\eta)\tilde{u}^\alpha(z^a,t)dz^1dz^2dz^3 \tag{11}$$

where

$$G(x^a,\eta) = (4\pi\eta)^{-3/2}exp[-\delta_{ab}x^ax^b/(4\eta)] \tag{12}$$

Here the Gaussian filter is expressed in normalized form so that

$$\int_\Omega G(x^a - z^a,\eta)dz^1dz^2dz^3 = 1 \tag{13}$$

For the case of bounded Ω we must impose boundary conditions for the filtered fields on $\partial\Omega$. The PDE filter, as it is defined here, will still be effective in damping out irresolvable fluctuations provided suitable boundary conditions can be imposed.

As η is increased from 0 each $\tilde{f}^\alpha \in \widehat{F}(M)$ may deviate from 0. We introduce

$$f^\alpha = \tilde{f}^\alpha + r^\alpha \tag{14}$$

for some residual $r^\alpha \in F(M)$ such that

$$r^\alpha|_{\eta=0} = 0 \tag{15}$$

Let $e^\alpha \in F(M)$ be defined by

$$e^\alpha = (\frac{\partial}{\partial\eta} - L)r^\alpha - \sigma^\alpha \tag{16}$$

where $\sigma^\alpha \in F(M)$ is given by

$$\sigma^\alpha = (L - U)\tilde{f}^\alpha \tag{17}$$

¿From (14), (16) and (17) is obtained

$$e^\alpha = (\frac{\partial}{\partial\eta} - L)f^\alpha - W\tilde{f}^\alpha \tag{18}$$

If $u^\alpha \in PDEF\{L,\tilde{f}^\alpha,\tilde{u}^\alpha\}$ then $\varphi^\alpha = 0$ and the vector field operator W vanishes. Hence for $u^\alpha \in PDEF\{L,\tilde{f}^\alpha,\tilde{u}^\alpha\}$

$$(\frac{\partial}{\partial\eta} - L)f^\alpha = e^\alpha \tag{19}$$

¿From (9) and (15) we have

$$f^\alpha|_{\eta=0} = 0 \tag{20}$$

Consider first the case $\Omega = \mathbf{R}^3$. We see that each f^α satisfies the initial value problem (19)-(20), where η replaces the traditional role taken by time and t appears only as a parameter. If each $e^\alpha \in F(M)$ is bounded on M the solution to this initial value problem can be obtained in the explicit form (see Lecture 8 [3])

$$f^\alpha(x^a, t, \eta) = \int_0^\eta \int_\Omega G(x^a - z^a, \eta - \xi) e^\alpha(z^a, t, \xi) dz^1 dz^2 dz^3 d\xi \tag{21}$$

Thus for consistency we need to generate residuals r^α such that, through the identity (16), each e^α is rendered sufficiently small.

If Ω has a boundary, $\partial\Omega$, then we can assume that given some prescription of u^α and r^α (and/or their spatial gradients) on the boundary $\partial\Omega$ we can set $f^\alpha|_{\partial\Omega} = 0$. This along with the system (19)-(20) defines an initial boundary value problem satisfied by each f^α. For an estimate of the consistency error we can replace the expression (21) by some inequality. For instance in terms of the $L_2(\Omega)$-norm, $\| \cdot \|$, we can obtain, for each $\alpha \in \{1, ..., N\}$, $\eta \in I$ and $t \in T$,

$$\| f^\alpha(\cdot, \eta) \| \leq \int_0^\eta \| e^\alpha(\cdot, \xi) \| e^{-\lambda(\eta - \xi)} d\xi \tag{22}$$

for some $\lambda > 0$. The inequality also holds for the case $\lambda = 0$.

If $e^\alpha = 0$ on M then the residuals r^α are known exactly. Thus, on M, the filtered fields of the solutions of the PDE (9) and the exact residuals $r^\alpha \in F(M)$ satisfy the system

$$\tilde{f}^\alpha + r^\alpha = 0 \tag{23}$$

$$(\frac{\partial}{\partial \eta} - L) r^\alpha - \sigma^\alpha = 0 \tag{24}$$

where σ^α is given by (17). These are the exact macroscopic equations for the filtered fields $u^\alpha \in PDEF\{L, \tilde{f}^\alpha, \tilde{u}^\alpha\}$. Written in this form it is clear where the difficulties arise in constructing subgrid scale models for general nonlinear PDE systems (9). In application one desires the solution computed only on some slice $M|_{\eta=const}$. The presence of the term $\partial r^\alpha / \partial \eta$ makes the solution of (24) impractical and some approximation for the residuals needs to be introduced. The task is to generate r^α such that e^α is minimzed in (16). The relationship (21) (or (22)) gives an estimate of how close (23) is satisfied by the filtered fields $u^\alpha \in PDEF\{L, \tilde{f}^\alpha, \tilde{u}^\alpha\}$ given any approximation of the residuals r^α.

3. Approximation of the Residuals

We consider an approximation to (24), presented in [1] and [2], that is valid for any slice $M|_{\eta=const}$ for $0 < \eta \leq \eta_0$. Assume $r^\alpha \in F(M)$, such that

$r^\alpha|_{\eta=0} = 0$, satisfy on M

$$(\frac{1}{\eta} - L)r^\alpha - \sigma^\alpha = 0 \tag{25}$$

for some $u^\alpha \in F(M)$, not necessarily in $PDEF\{L, \widetilde{f}^\alpha, \widetilde{u}^\alpha\}$, and σ^α given by (17). A calculation based on (15), (16) and (25) gives

$$e^\alpha = \frac{\partial r^\alpha}{\partial \eta} - \frac{1}{\eta}(r^\alpha - r^\alpha|_{\eta=0}) = \frac{\eta}{2}\frac{\partial^2 r^\alpha}{\partial \eta^2}|_{\eta=\xi}, \qquad \xi \in (0, \eta) \tag{26}$$

If $\partial^2 r^\alpha / \partial \eta^2$ can be suitably bounded then we have $e^\alpha = O(\eta)$. ¿From (21) (or (22)) it follows that $f^\alpha = O(\eta^2)$ for $u^\alpha \in PDEF\{L, \widetilde{f}^\alpha, \widetilde{u}^\alpha\}$.

In general any $u^\alpha \in PDEF\{L, \widetilde{f}^\alpha, \widetilde{u}^\alpha\}$ will not satisfy (23) exactly on M if the residuals are not exact, i.e. they do not satisfy (24). In application one generates $u^\alpha \in F(M)$ by enforcing (23) and introducing some approximation for the residuals r^α (for example obtained from (25)). In such a case each u^α can only approximate members of $PDEF\{L, \widetilde{f}^\alpha, \widetilde{u}^\alpha\}$.

4. Approximation of the Filtered Fields

Let $u^\alpha \in F(M)$ satisfy (i) and (iii) of Definition 2 and be generated from (23) given some approximation of the residuals r^α (for example through (25)). Let $\bar{u}^\alpha \in PDEF\{L, \widetilde{f}^\alpha, \widetilde{u}^\alpha\}$. Since u^α is not a member of $PDEF\{L, \widetilde{f}^\alpha, \widetilde{u}^\alpha\}$ there exists $\varphi^\alpha \in F(M)$ satisfying (2) and we have

$$(\frac{\partial}{\partial \eta} - L)(u^\alpha - \bar{u}^\alpha) = \varphi^\alpha \tag{27}$$

Consider first the case Ω is unbounded (i.e. $\Omega = \mathbf{R}^3$). If $\varphi^\alpha \in F(M)$ is bounded on M then we obtain

$$(u^\alpha - \bar{u}^\alpha)(x^a, t, \eta) = \int_0^\eta \int_\Omega G(x^a - z^a, \eta - \xi)\varphi^\alpha(z^a, t, \xi) dz^1 dz^2 dz^3 d\xi \tag{28}$$

For the case where Ω has a boundary $\partial\Omega$ we assume that $u^\alpha|_{\partial\Omega} = \bar{u}^\alpha|_{\partial\Omega}$. As before, in terms of the $L_2(\Omega)$-norm we can obtain, for each $\alpha \in \{1, ..., N\}$, $\eta \in I$ and $t \in T$,

$$\| (u^\alpha - \bar{u}^\alpha)(\cdot, \eta) \| \leq \int_0^\eta \| \varphi^\alpha(\cdot, \xi) \| e^{-\lambda(\eta - \xi)} d\xi \tag{29}$$

for some $\lambda > 0$. The inequality also holds for the case $\lambda = 0$. Both (28) and (29) suggest that convergence of the approximations of the filtered fields rests upon the boundedness of φ^α.

A calculation based on (16), (17) and (23) gives

$$W\tilde{f}^{\alpha} = -e^{\alpha} \tag{30}$$

If the residuals r^{α} are exact, then $e^{\alpha} = 0$ and $W\tilde{f}^{\alpha} = 0$. For this to hold for arbitrary $\tilde{f}^{\alpha}$ we must have $W = 0$ (the zero operator). Hence $\varphi^{\alpha} = 0$ and $u^{\alpha} \in PDEF\{L, \tilde{f}^{\alpha}, \tilde{u}^{\alpha}\}$. If each r^{α} is not exact then each u^{α}, generated from (23), will not be a filtered field and each φ^{α} will not vanish everywhere on M. Suppose that approximations for the residuals, r^{α}, can be found rendering each $e^{\alpha} = O(\delta(\eta))$, where δ is an order function with respect to η such that $lim_{\eta\to 0}\delta(\eta) = 0$. The problem is then transformed into one of establishing the rate at which the operator W tends to the zero operator as $\eta \to 0$.

5. Example: Reactive Flows

The ideas of the previous sections are developed in the context of general nonlinear PDE. For demonstration purposes we assume an incompressible fluid. The $\tilde{f}^{a}$ are associated with the three fluid momentum equations and $\tilde{f}^{n-1}$ is associated with the continuity or fluid mass conservation equation. The system is augmented with $\tilde{f}^{n-1+A}$ $(A = 1, ..., Q)$ associated with Q mass balance equations for the Q chemical components. In this case we have $N = n - 1 + Q$ and

$$u^{a} = v^{a}, \quad u^{n-1} = p, \quad u^{n-1+A} = \omega^{A}, \quad (A = 1, ..., Q) \tag{31}$$

where v^{a} $(1 \leq a \leq 3)$ correspond to the fluid velocity components, p the fluid pressure and ω^{A} $(A = 1, ..., Q)$ are the mass fractions of the chemical components. We can write the functions $\tilde{f}^{\alpha} \in \widehat{F}(M)$ corresponding to the equations of motion of an incompressible fluid and chemical component mass balance as

$$\begin{aligned}
\tilde{f}^{a} &= v^{a}_{,t} + (v^{b}v^{a} + \delta^{ab}p - \delta^{bc}v^{a}_{,c}/Re)_{,b} \\
\tilde{f}^{n-1} &= v^{b}_{,b} \\
\tilde{f}^{n-1+A} &= \omega^{A}_{,t} + (v^{b}\omega^{A} - \kappa\delta^{bc}\omega^{A}_{,c})_{,b} + \xi^{A}
\end{aligned} \tag{32}$$

where Re is the Reynolds number, κ is a coefficient associated with molecular diffusion of the chemical components in the fluid medium and $\xi^{A} = \xi^{A}(\omega^{1}, ..., \omega^{Q})$ are the chemical source terms. It should be mentioned that to regard (9) under the prescription (32) as an exact description of the system at $\eta = 0$ is not entirely true since the fluid viscous and chemical diffusion terms are only approximate models of nonlinear effects ocurring at even smaller scales. For the sake of this demonstration we shall regard this formulation as representing the exact microscopic equations at $\eta = 0$. We should note that the viscous and diffusion terms are linear and do not contribute to the residuals under filtering.

A calculation based on (17) and (32) leads to

$$\begin{aligned} \sigma^{a} &= 2\delta^{cd}(v^{b}_{,c}v^{a}_{,d})_{,b} \\ \sigma^{n-1} &= 0 \\ \sigma^{n-1+A} &= 2\delta^{cd}(v^{b}_{,c}\omega^{A}_{,d})_{,b} + \Xi^{A} \end{aligned} \tag{33}$$

where

$$\Xi^{A} = (L - U)\xi^{A} \tag{34}$$

is left in the generic form since we have not specified the source terms ξ^A as explicit functions of the chemical components. We can assume that the source terms $\xi^A \in \widehat{F}(M)$.

The identities (33) provide the source terms that appear in the system (23)-(24) (or the approximate system (23), (25)). Since $\sigma^{n-1} = 0$ we can set $r^{n-1} = 0$ in (16) and hence the continuity equation will be invariant under filtering, i.e. $\widetilde{f}^{n-1} = 0$ on M. It is seen that each σ^a, for the incompressible case, depend only on the velocities and their spatial partial derivatives. The corresponding residuals, r^a, will model the influence of the residual stress/strain of the turbulent fluid.

The source terms σ^{n-1+A} can be decomposed into two parts

$$\sigma^{n-1+A} = \sigma^{n-1+A}_{disp} + \sigma^{n-1+A}_{reac} \tag{35}$$

where σ^{n-1+A}_{disp} is associated with dispersion and σ^{n-1+A}_{reac} is associated with the reaction kinetics. In the absence of reaction source terms (i.e. when $\xi^A = 0$) each σ^{n-1+A}_{reac} vanish and the residuals, r^{n-1+A}, will model the influence of the dispersion of the chemical components in the flow field.

References

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